HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For

Polyethylbenzene Bottoms

CAS Number 68987-42-8

Prepared by:

American Chemistry Council
Ethylbenzene Panel

December 4, 2003

EXECUTIVE SUMMARY

The Ethylbenzene Panel (Panel) of the American Chemistry Council and the Panel's member companies who produce Polyethylbenzene Bottoms (CAS number 68987-42-8) have committed to developing screening level human health, environmental effects and fate, and physicochemical data for Polyethylbenzene Bottoms under the Environmental Protection Agency's (EPA's) High Production (HPV) Challenge Program (Program). The Polyethylbenzene Bottoms stream is a co-product of ethylbenzene manufacture and a Class II complex mixture. Since no published data were found and limited unpublished studies were found for HPV endpoints, the screening level studies as listed in Section IV will be conducted. Since this material is unique to the ethylbenzene manufacturing process and does not have a composition common with other HPV materials, it is not feasible to combine this material into a category combining multiple CAS numbers for hazard assessment or HPV testing.

Ethylbenzene Panel

Producers of Polyethylbenzene Bottoms

ATOFINA Petrochemicals Inc.

BP Amoco Chemical Company

Chevron Phillips Chemical Company LP

The Dow Chemical Company

Lyondell Chemical Company

NOVA Chemicals Inc.

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I. INTRODUCTION

The Ethylbenzene Panel (Panel) of the American Chemistry Council and the Panel's member companies who produce Polyethylbenzene Bottoms (PEB HPV Task Group) have committed to develop screening level human health, environmental effects and fate, and physicochemical data for Polyethylbenzene Bottoms under the Environmental Protection Agency's (EPA's) High Production (HPV) Challenge Program (Program).

In preparing this test plan, the PEB HPV Task Group has given careful consideration to the principles contained in the letter EPA sent to all HPV Challenge Program participants on October 14, 1999. As directed by EPA in that letter, the Panel has conducted a thorough search for existing data and a thoughtful, qualitative analysis of the adequacy of existing data. The Panel has taken the same thoughtful approach when developing its test plan. The Panel believes its test plan conforms to the principles articulated in EPA's letter.

The Panel conducted a search of the published literature and found no test data on this material. Panel members searched company files for unpublished data and found data on endpoints that are not part of the HPV dataset (e.g. irritation) or the data were not sufficiently robust to meet the standards of the HPV program. The Panel also considered whether this material could be combined in a category with other HPV chemicals for purposes of the HPV program, but since this material is unique to the ethylbenzene manufacturing process and does not have a composition common with other HPV materials, it is not feasible to combine this material into a category combining multiple CAS numbers for hazard assessment or HPV testing.

Polyethylbenzene Bottoms is identified by CAS number 68987-42-8. No adequate existing data were found in the published literature. Limited data applicable to the HPV endpoints were obtained in the form of unpublished reports sponsored by the producers. The objective of the Panel's participation in the HPV program is to identify and develop sufficient test data and/or other information to adequately characterize the human and environmental fate for the category in accordance with the EPA HPV Program. The Panel plans to conduct tests to develop the screening level data.

II. DESCRIPTION OF POLYETHYLBENZENE BOTTOMS

The Polyethylbenzene Bottoms stream is a co-product of ethylbenzene manufacture. Ethylbenzene is produced through alkylation of benzene with ethylene. In addition to the production of ethylbenzene, there are side reactions that involve the reaction of ethylene with ethylbenzene to produce diethylbenzene and further alkylations to produce triethylbenzene and polyethylbenzene. In addition, butylbenzene and other alkylaromatics may be formed in varying

amounts. After the ethylbenzene is removed, the remaining stream is separated into a diethylbenzene-rich stream and a bottoms stream. This co-product bottoms stream is described as Benzene, ethylenated, residues (CAS# 68987-42-8), also called Polyethylbenzene Bottoms or Polyethylbenzene Residue. This material is a Class II complex mixture.

Chemical Name	Other Names	CAS #
Benzene, ethylenated, residues	Polyethylbenzene Bottoms Polyethylbenzene Residue PEB Bottoms PEB Residue	68987-42-8

The composition of Polyethylbenzene Bottoms listed below is based on capillary GC analysis of samples submitted by the eight participating companies to BP Amoco Analytical Technology (BP Amoco, 2000).

Composition	Wt%
Diphenylethanes	15 – 32
Diphenylmethanes	<0.5 – 31
Other diphenylalkanes	7 –17
Ethyl diphenylethanes & diethylbiphenyls	9 –21
Polyethylbenzenes	<0.1 – 19
Triethylbenzenes	<1 – 26
Diethylbenzenes (m-, o-, p-)	<0.1 –4
Butylbenzenes	<0.1
Other alkylbenzenes	9 – 24
PNAs (3-ring)	0.4 – 11
Ethylbenzene	<0.1
Benzene	<0.1
Paraffins/Naphthenes	<0.3
Total of unidentified components each present at <0.1%	3 – 5

Please note that the Diethylbenzene Rich-Streams (CAS Registry #25340-17-4 and 68608-82-2) are currently being tested separately in 2003 under the HPV Chemical Program.

III. SUMMARY OF EXISTING INFORMATION

No published data on Polyethylbenzene Bottoms for HPV endpoints were found following a search of the literature. Although some unpublished reports on some acute studies were reviewed, none of these data were considered adequate for the HPV endpoints. Nonetheless, robust summaries are provided. Polyethylbenzene Bottoms is characterized by low acute oral and dermal toxicity. The acute oral LD_{50} for rats was greater than 5.0 g/kg (Gulf Life Sciences

Center, 1985a). Dermal application at 1.0 or 2.0 g/kg on five consecutive days to rats resulted in no mortality (Gulf Life Sciences Center, 1985b); body weights were decreased at both dose levels.

IV. TEST PLAN

A sample representing industry production will be tested. Equal quantities of a Polyethylbenzene Bottoms samples obtained from each current producer company will be blended to produce the Polyethylbenzene Bottoms test stream. The composition of the stream will be characterized and the following studies conducted:

Test	Method
Melting Point/Melting Point Range	**OECD 102**
Boiling Point	**OECD 103**
Vapor Pressure	**OECD 104**
Water Solubility	**OECD 105**
Partition Coefficient (n-octanol/water, shake flask method)	**OECD 107**
Photodegradation	**(Technical Discussion)**
Fugacity Model I or III	**(Model)**
Ready Biodegradability: Manometric Respirometry Test	**OECD 301 F**
Fish Acute Toxicity Test	**OECD 203**
***Daphnia* sp., Acute Immobilization Test and Reproduction Test**	**OECD 202**
Algae, Acute Growth Inhibition Test	**OECD 201**
Bacterial Reverse Mutation Test	**OECD 471**
***In vitro* Mammalian Chromosome Aberration Test**	**OECD 473**
Combined Repeated Dose Toxicity Study with Reproductive/Developmental Toxicity Screening Test	**OECD 422**
Hydrolysis	**(Technical Discussion)**

The chemical composition of the Polyethylbenzene Bottoms streams indicates this stream is not subject to hydrolysis at measurable rates. Therefore, information for this endpoint will be summarized in a technical review document.

V. REFERENCES

BP Amoco Company, 2000. Unpublished Report for the American Chemistry Council Ethylbenzene Panel (CMA Reference No. EB-60-RES-HPV-BP Amoco). June 7, 2000). BP Amoco Technology Center, Naperville, IL.

Gulf Life Sciences Center. 1985a. Acute oral toxicity study in rats of Polyethylbenzene Bottoms. Project No. 84-2133. Sponsored by Gulf Oil Products Company. Gulf Life Sciences Center, Pittsburgh, PA.

Gulf Life Sciences Center. 1985b. Five-day repeated dose dermal toxicity in rats of Polyethylbenzene Bottoms. Project No. 84-2137. Sponsored by Gulf Oil Products Company. Gulf Life Sciences Center, Pittsburgh, PA.

Table 1. Assessment Plan for Polyethylbenzene Bottoms. (Robust summaries provided separately)

	Human Health Effects						Ecotoxicity				Environmental Fate			
Stream Description	**Acute Toxicity**	**Genetic Point Mut.**	**Genetic Chrom.**	**Sub-chronic**	**Develop-mental**	**Reproduc-tion**	**Acute Fish**	**Acute Invert.**	**Algal Toxicity**	**Physical Chem.**	**Photo-deg.**	**Hydro-lysis**	**Fugacity**	**Biodeg.**
Polyethylbenzene Bottoms	E	T	T	T	T	T	T	T	T	T	TD	TD	M	T

E Existing Data
T Testing proposed
TD Technical Discussion
M Model